

Triisopropanolamine
122-20-3 | DTXSID5021415

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 302 °C

Global applicability domain: Outside

Local applicability domain index: 2.62e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Triisopropanolamine</div> <div>Measured: 305</div> <div>Predicted: 302</div>	<div>Image not found</div> <div>Triethanolamine</div> <div>Measured: 335</div> <div>Predicted: 326</div>	<div>Image not found</div> <div>Metaraminol</div> <div>Measured: 218</div> <div>Predicted: 257</div>
<div>Image not found</div> <div>Diisopropanolamine</div> <div>Measured: 250</div> <div>Predicted: 248</div>	<div>Image not found</div> <div>N-Butyldiethanolamine</div> <div>Measured: 275</div> <div>Predicted: 265</div>	